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**From:** Strynar, Mark [Strynar.Mark@epa.gov]  
**Sent:** 4/16/2020 12:51:40 PM  
**To:** Liberatore, Hannah [Liberatore.Hannah@epa.gov]; Miller, Kelsey [Miller.Kelsey@epa.gov]; McCord, James [mccord.james@epa.gov]  
**Subject:** Fw: in vivo PFAS Studies  
**Attachments:** Bao2020\_HFPO\_oligomeracids\_PFOAalternatives.pdf; 1-s2.0-S1385894719322764-mmc1.docx

Not sure if you all have seen this paper.

Mark

Dr. Mark Strynar  
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**From:** Smeltz, Marci <smeltz.marci@epa.gov>  
**Sent:** Thursday, April 16, 2020 8:17 AM  
**To:** Strynar, Mark <Strynar.Mark@epa.gov>  
**Subject:** RE: in vivo PFAS Studies

Hi Mark,

I'm glad I gave you the scoop. Always want to include you in all things PFAS if I can!

The HFPO acids were the ones from last summer that I tried to analyze. When opening the DMSO stock bottle, it provided a horrible smell and of course didn't show anything in MS2. So, I agree it is very nasty in many ways. I think Barbara is trying to procure this compound neat for easier analysis and for better preparation/solubilization for assay needs. I'll be sure to consult with Hannah (and look over the manuscript draft she gave me) to decide how best to proceed.

There is also talk that we may start trying to do some metabolite ID studies, and I will likely be included. It makes me happy to be able to revisit some of previous types of research I did at my old job and also get a better grasp on NTA workflows. Guess this could also include doing some stability studies too, which could be a nice overlap with what Hannah is completing.

I'd be more than glad to chat whenever we get back to normal and keep you informed of findings. I'm including a paper (and SI) from a group in China printed early this year on the effect of molecular structure for these HFPO oligomer acids and degradation pathways (Bao et al).

Take care,  
Marci

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**From:** Strynar, Mark <Strynar.Mark@epa.gov>  
**Sent:** Thursday, April 16, 2020 7:16 AM

To: Smeltz, Marci <smeltz.marci@epa.gov>

Subject: Re: in vivo PFAS Studies

Hi Marci,

Thanks for sharing. On slide 11 the HFPO-trimer acid seems to be the second chemical shown. I am told this is a pretty nasty compound. I look forward to seeing what you all find out. I am also sure if this was put in DMSO it would turn into the E2 compound very quickly. To study it you will need to be sure to make it up in another solvent. Perhaps Hannahs work can help define what solvent is best. If put in methanol you can get losses to a methyl ester however I am not sure if you can alwso get and ethyl ester loss if stored in ethanol. I expect that can happen as well.

No one has approached me at all about any of this. When we get back to work I am happy to help out on this front. I hope you are staying safe at this time as well.

Mark

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From: Smeltz, Marci <smeltz.marci@epa.gov>

Sent: Monday, April 13, 2020 1:41 PM

To: Strynar, Mark <[Strynar.Mark@epa.gov](mailto:Strynar.Mark@epa.gov)>

Subject: in vivo PFAS Studies

Hi Mark,

I'm sure you've been made aware that our division (CCTE-CCED) under DeVito is planning to do some in vivo PFAS work. Attached is a PowerPoint from February when a lot of these projects were first discussed as a division. I wanted to share the list of compounds, as many you are likely very interested in (from previously published research), and what type of work is going to be completed.

PFAS Information		Planned Studies	MS Method
DTXSID70191136	Perfluoro-3-methoxypropanoic acid	5 day in vivo study at JTI; in vitro plasma protein binding; In vitro hepatic clearance	LC-MS (method already prepared; PFPE-2)
DTXSID70276659	Perfluoro-(2,5,8-trimethyl-3,6,9-trioxadodecanoic)acid	5 day in vivo study at JTI; in vitro plasma protein binding; In vitro hepatic clearance	LC-MS (no method yet – one of the two <i>smelly</i> compounds from last summer's method dev.)
DTXSID00190950	6:1 Fluorotelomer alcohol	5 day in vivo study at JTI; in vitro plasma protein binding; In vitro hepatic clearance	GC-MS (Amanda Brennan to complete analysis/Matt Henderson and Scott Clifton may have methods)
DTXSID9037743	10:2 Fluorotelomer acrylate	5 day in vivo study at JTI; in vitro plasma protein binding; In vitro hepatic clearance	GC-MS (Amanda Brennan to complete analysis/Matt

			Henderson and Scott Clifton may have methods)
DTXSID30892354	Perfluoro-3,6-dioxo-4-methyl-7-octene-1-sulfonic acid	5 day in vivo study at EPA; in vitro plasma protein binding; In vitro hepatic clearance	LC-MS (no method; pote)
DTXSID50884231	2,4-Dimethyl-1-(1-phenylethyl)benzene	5 day in vivo study at EPA; in vitro plasma protein binding; In vitro hepatic clearance	GC-MS (positive control of sorts?; not PFAS)
DTXSID00408562	PFMOAA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID50892351	PFO2HxA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID20892348	PFO3OA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID90723993	PFO4DA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID50723994	PFO5DA (PFO5DoA)	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID10892352	Byproduct 2 (BP2)	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID60896486	PEPA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID80528474	PMPA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID60904459	Hydro-EVE Acid	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID80904754	NVHOS	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (use McCord 2018 as ref)
DTXSID70880215	HFPO-DA	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (method already prepared)
DTXSID8037708	PFOA-NH <sub>4</sub>	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (method already prepared)
DTXSID8037706	PFOS-K	Cape Fear in vivo study at EPA; in vitro tox work likely (may even do some assays as mixtures)	LC-MS (method already prepared)

I'm not sure of the exact breakdown of who is running which samples/sets by LC-MS. Denise MacMillan is the other assigned individual (for the in vivo samples, at least). Not sure if she has dropped you any notes about these.

Do you have any insight or concerns? Are there other studies or information that you are wanting to know that would not be too farfetched to complete (from an in vitro side at least)? I'm not 100% sure what tissues/fluids will be collected from the rat studies, but can find out if you're interested.

My biggest compound of concern is Perfluoro-(2,5,8-trimethyl-3,6,9-trioxadodecanoic)acid (HFPO-TeA). I never was able to successfully tune it or get good confirmatory fragments from the stocks in DMSO. We were also provided in EtOH, but time got away and I never really got to investigate as much as I'd like. I did run MS full scans for both solvents (ESI pos and ESI neg) and saw a peak in EtOH stock only, but couldn't piece it back together well; it is on my to do list to review again. This compound should behave like GenX and decarboxylate in DMSO and not EtOH? Whenever we do get back to normal life, I am planning to try to make these methods work either on the TQ-S micro in D278 or the new TQ-XS. I have a few papers that your friend from Chemours had sent you over the summer and plan to see if any other literature exists.

Hope you and your family are doing well in these crazy times.

Take care,

Marci

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**Marci Smeltz, Ph.D.**

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